EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	0	"514359".ccls.	US-PGPUB; USPAT	OR	OFF	2007/11/29 14:13
L2	711	"514/359".ccls.	US-PGPUB; USPAT	OR	OFF	2007/11/29 14:13
L3	171	"514/359".ccls. and 548/255.ccls.	US-PGPUB; USPAT	OR	OFF	2007/11/29 14:13
L4	125	"514/359".ccls. and 548/255.ccls. and triazole	US-PGPUB; USPAT	OR	OFF	2007/11/29 14:13
S1	11	"1914954"	USPAT; EPO; JPO; DERWENT	OR	OFF	2007/11/29 14:12
S2	1	("6632815").PN.	USPAT; USOCR	OR	OFF	2007/11/29 12:21
S3	1	("4233059").PN.	USPAT; USOCR	OR	OFF	2007/11/29 12:34
S4	1	("7265227").PN.	USPAT; USOCR	OR	OFF	2007/11/29 13:51
S5	0	("7307090").PN.	USPAT; USOCR	OR	OFF	2007/11/29 13:51

```
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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page for STN Seminar Schedule - N. America
 NEWS  2  JUL 02   LMEDLINE coverage updated
 NEWS  3  JUL 02   SCISEARCH enhanced with complete author names
 NEWS  4  JUL 02   CHEMCATS accession numbers revised
 NEWS  5  JUL 02   CA/CAplus enhanced with utility model patents from China
 NEWS  6  JUL 16   CAplus enhanced with French and German abstracts
 NEWS  7  JUL 18   CA/CAplus patent coverage enhanced
 NEWS  8  JUL 26   USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS  9  JUL 30   USGENE now available on STN
 NEWS 10  AUG 06   CAS REGISTRY enhanced with new experimental property tags
 NEWS 11  AUG 06   FSTA enhanced with new thesaurus edition
 NEWS 12  AUG 13   CA/CAplus enhanced with additional kind codes for granted
                   patents
 NEWS 13  AUG 20   CA/CAplus enhanced with CAS indexing in pre-1907 records
 NEWS 14  AUG 27   Full-text patent databases enhanced with predefined
                   patent family display formats from INPADOCDB
 NEWS 15  AUG 27   USPATOLD now available on STN
 NEWS 16  AUG 28   CAS REGISTRY enhanced with additional experimental
                   spectral property data
 NEWS 17  SEP 07   STN AnaVist, Version 2.0, now available with Derwent
                   World Patents Index
 NEWS 18  SEP 13   FORIS renamed to SOFIS
 NEWS 19  SEP 13   INPADOCDB enhanced with monthly SDI frequency
 NEWS 20  SEP 17   CA/CAplus enhanced with printed CA page images from
                   1967-1998
 NEWS 21  SEP 17   CAplus coverage extended to include traditional medicine
                   patents
 NEWS 22  SEP 24   EMBASE, EMBAL, and LEMBASE reloaded with enhancements
 NEWS 23  OCT 02   CA/CAplus enhanced with pre-1907 records from Chemisches
                   Zentralblatt
 NEWS 24  OCT 19   BEILSTEIN updated with new compounds
 NEWS 25  NOV 15   Derwent Indian patent publication number format enhanced
 NEWS 26  NOV 19   WPIX enhanced with XML display format

 NEWS EXPRESS  19 SEPTEMBER 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 07:58:22 ON 29 NOV 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 07:58:33 ON 29 NOV 2007
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STRUCTURE FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2
DICTIONARY FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
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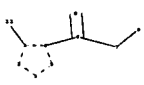


chain nodes :
6 7 8 9 11
ring nodes :
1 2 3 4 5

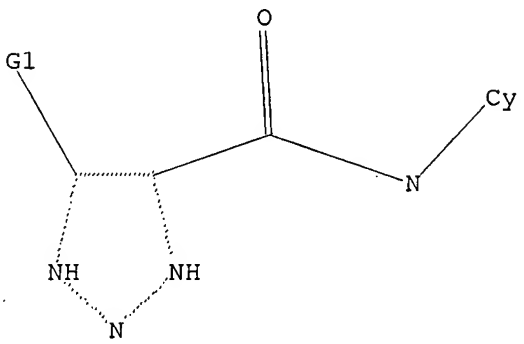
chain bonds :
3-11 4-6 6-7 6-8 7-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 6-7 6-8 7-9
exact bonds :
4-6

G1:X,Ak,CH3,CN,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 11:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 X,Ak,Me,CN,NO2

Structure attributes must be viewed using STN Express query preparation.

=> fil reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.45 0.66

FILE 'REGISTRY' ENTERED AT 07:59:03 ON 29 NOV 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2
DICTIONARY FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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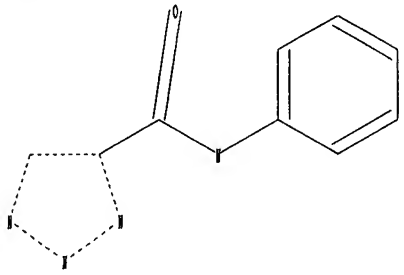
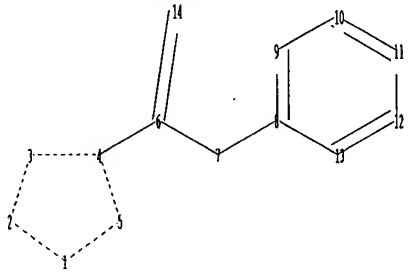


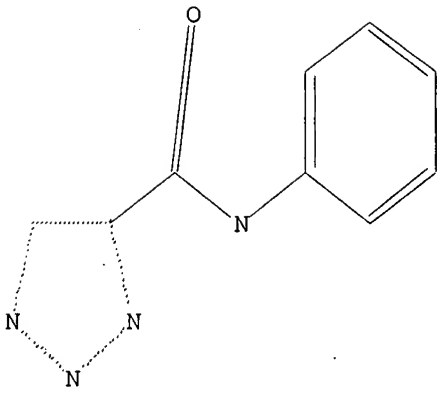


chain nodes :
6 7 14
ring nodes :
1 2 3 4 5 8 9 10 11 12 13
chain bonds :
4-6 6-7 6-14 7-8
ring bonds :
1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-14 7-8
exact bonds :
4-6
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS

L2 STRUCTURE UPLOADED

=> d
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l2
SAMPLE SEARCH INITIATED 07:59:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 372 TO ITERATE

100.0% PROCESSED 372 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 6283 TO 8597
PROJECTED ANSWERS: 4597 TO 6603

L3 50 SEA SSS SAM L2

=> s l2 full
FULL SEARCH INITIATED 07:59:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7056 TO ITERATE

100.0% PROCESSED 7056 ITERATIONS 5071 ANSWERS
SEARCH TIME: 00.00.01

L4 5071 SEA SSS FUL L2

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 172.76

FILE 'CAPLUS' ENTERED AT 07:59:23 ON 29 NOV 2007
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FILE COVERS 1907 - 29 Nov 2007 VOL 147 ISS 23
FILE LAST UPDATED: 28 Nov 2007 (20071128/ED)

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http://www.cas.org/infopolicy.html

=> s l4
L5   159 L4

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.35	175.11

FILE 'REGISTRY' ENTERED AT 08:02:11 ON 29 NOV 2007
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STRUCTURE FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2
DICTIONARY FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2

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  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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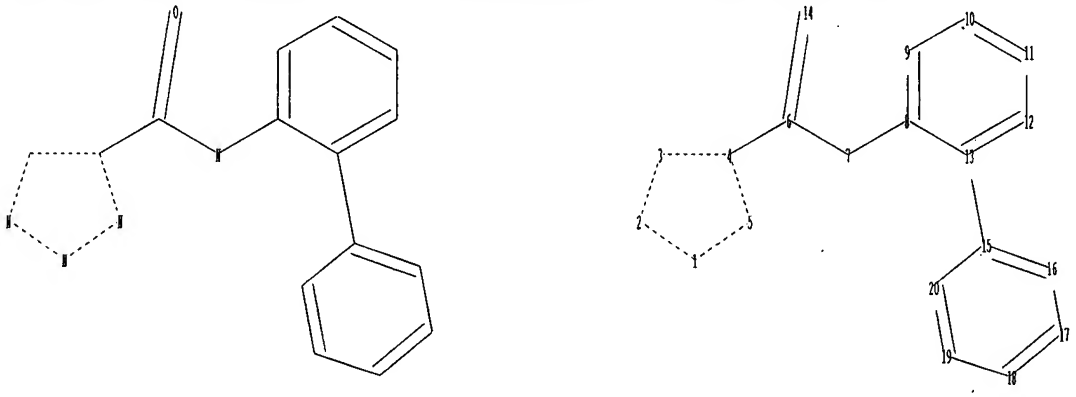
Uploading C:\Program Files\Stnexp\Queries\10524721c.str



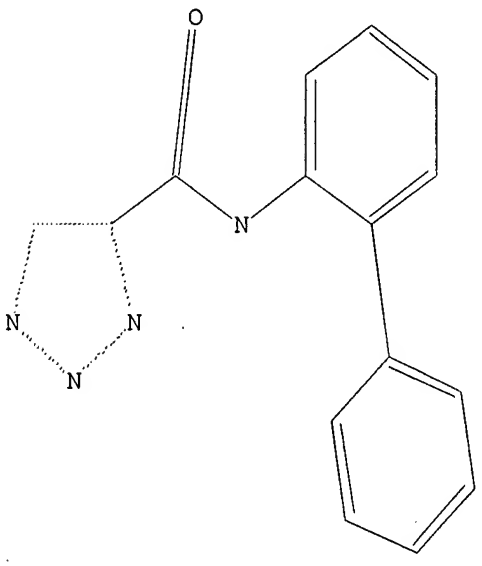
chain nodes :
6 7 14
ring nodes :
1 2 3 4 5 8 9 10 11 12 13 15 16 17 18 19 20

chain bonds :
4-6 6-7 6-14 7-8 13-15
ring bonds :
1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20 16-17
17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-14 7-8
exact bonds :
4-6 13-15
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom

L6 STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l6
SAMPLE SEARCH INITIATED 08:02:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 3 TO 163

```
L7             3 SEA SSS SAM L6

=> s l6 full
FULL SEARCH INITIATED 08:02:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       38 TO ITERATE

100.0% PROCESSED       38 ITERATIONS                          22 ANSWERS
SEARCH TIME: 00.00.01

L8            22 SEA SSS FUL L6

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     172.10     347.21

FILE 'CAPLUS' ENTERED AT 08:02:33 ON 29 NOV 2007
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FILE COVERS 1907 - 29 Nov 2007  VOL 147 ISS 23
FILE LAST UPDATED: 28 Nov 2007  (20071128/ED)

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They are available for your review at:

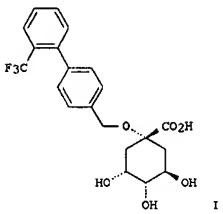
http://www.cas.org/infopolicy.html

=> s l8
L9             2 L8

=> d ibib abs hitstr tot
```

L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:441839 CAPLUS
DOCUMENT NUMBER: 143:153207
TITLE: Quinic Acid Derivatives as Sialyl Lewisx-Mimicking Selectin Inhibitors: Design, Synthesis, and Crystal Structure in Complex with E-Selectin
AUTHOR(S): Kaila, Neelu; Somers, William S.; Thomas, Bert E.; Thakker, Paresh; Janz, Kristin; DeBernardo, Silvano; Tam, Steve; Moore, William J.; Yang, Ruiyang; Wrona, Wojciech; Bedard, Patricia W.; Crommie, Deidre; Keith, James C., Jr.; Tsao, Desiree H. H.; Alvarez, Juan C.; Ni, Heyu; Marchese, Erik; Patton, John T.; Magnani, John L.; Camphausen, Raymond T.
CORPORATE SOURCE: Chemical Screening Sciences and Cardiovascular and Metabolic Disease Research, Wyeth, Cambridge, MA, 02140, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(13), 4346-4357
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:153207
GI



I

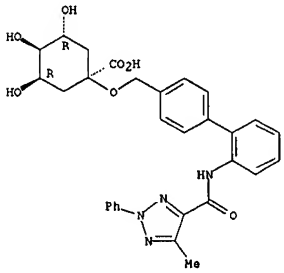
AB A search for noncarbohydrate sLex mimics led to the development of quinic acid derivs. as selectin inhibitors. At Wyeth the first cocrystal structure of a small mol., quinic acid, with E-selectin was solved. In the cocomplex two hydroxyls of quinic acid mimic the calcium-bound fucose of the tetrasaccharide sLex. The x-ray structure, together with structure based computational methods, was used to design quinic acid based libraries that were synthesized and evaluated for their ability to block the interaction of sLex with P-selectin. A large number of analogs were prepared using solution-phase parallel synthesis. Selected compds. showed decrease in leukocyte rolling in the IVM mouse model. I inhibited neutrophil influx in the murine TIP model and demonstrated good plasma exposure.

IT 859225-04-0P
RL: CPN (Combinatorial preparation); SPN (Synthetic preparation); CMBI (Combinatorial study); PREP (Preparation)
(preparation of a combinatorial library of quinic acid derivs. as sialyl Lewisx-mimicking selectin inhibitors including the design, and crystal

L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
structure in complex with E-selectin)

RN 859225-04-0 CAPLUS
CN Cyclohexanecarboxylic acid, 3,4,5-trihydroxy-1-[[2'-[[(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)carbonyl]amino][1,1'-biphenyl]-4-yl]methoxy]-, (3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

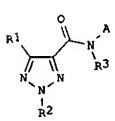
ACCESSION NUMBER: 2004:182852 CAPLUS
DOCUMENT NUMBER: 140:235719
TITLE: Preparation of triazolylcarboxylic acid derivatives with antifungal activity for agricultural use
INVENTOR(S): Ehrenfreund, Josef; Tobler, Hans; Walter, Harald
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018438	A2	20040304	WO 2003-EP9111	20030818
WO 2004018438	A3	20040826		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2494263	A1	20040304	CA 2003-2494263	20030818
AU 2003253417	A1	20040311	AU 2003-253417	20030818
EP 1539717	A2	20050615	EP 2003-792351	20030818
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003013686	A	20050621	BR 2003-13686	20030818
CN 1678593	A	20051005	CN 2003-819890	20030818
JP 2006502244	T	20060119	JP 2005-501204	20030818
EG 23485	A	20051205	EG 2003-821	20030820
IN 2004CN03147	A	20060217	IN 2004-CN3147	20041231
MX 2005PA01819	A	20050419	MX 2005-PA1819	20050215
US 2006154967	A1	20060713	US 2005-524721	20050216

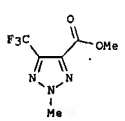
PRIORITY APPLN. INFO.:

GB 2002-19612	A	20020822
GB 2003-10464	A	20030507
WO 2003-EP9111	W	20030818

OTHER SOURCE(S): MARPAT 140:235719
GI



I



II

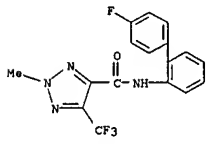
AB Title compds. I [A = ortho-substituted aryl or heteroaryl ring system; R1 = halo, CN, NO2, alkyl, haloalkyl, alkoxy, haloalkoxy, (un)substituted alkene, etc.; R2 = alkyl, haloalkyl, alkoxyalkyl, etc.; R3 = H,

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

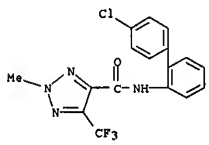
(un)substituted-alkyl, -propargyl, -alkoxy, etc.] were prepd. and disclosed as having antifungal activity. Thus, e.g., II was prepd. via methylation of 1,2,3-triazole-4,5-dicarboxylic acid di-Me ester, with subsequent monohydrolysis and fluorination of the carboxylic acid moiety to the trifluoromethyl moiety. I were tested against 9 different agriculturally relevant fungi with varying degrees of efficacy obsd. Addnl., a compn. of I with a suitable carrier for controlling microorganisms and preventing attack and infestation of plants therewith is claimed.

IT 668491-33-6P 668491-34-7P 668491-35-8P
668491-36-9P 668491-37-0P 668491-45-0P
668491-46-1P 668491-47-2P 668491-48-3P
668491-49-4P 668491-50-7P 668491-51-8P
668491-52-9P 668491-56-3P 668491-61-0P
668491-62-1P 668491-63-2P 668491-64-3P
668491-68-7P 668491-69-8P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of triazolylcarboxylic acid derivs. with antifungal activity)

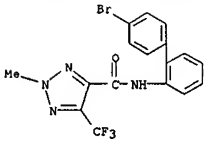
RN 668491-33-6 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-fluoro[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



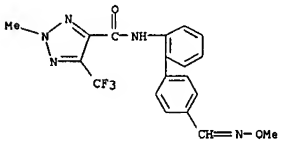
RN 668491-34-7 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-chloro[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



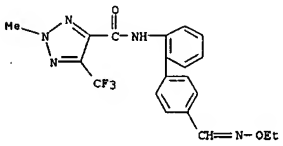
RN 668491-35-8 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-bromo[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



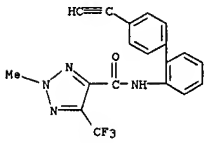
RN 668491-36-9 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-[4'-[(methoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



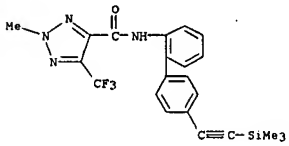
RN 668491-37-0 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-[4'-[(ethoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



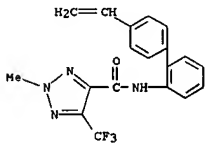
RN 668491-45-0 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethynyl[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



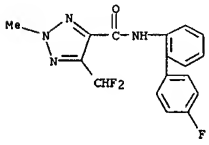
RN 668491-46-1 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 2-methyl-5-(trifluoromethyl)-N-[4'-[(trimethylsilyl)ethynyl][1,1'-biphenyl]-2-yl]- (9CI) (CA INDEX NAME)



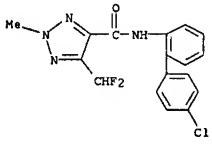
RN 668491-47-2 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethenyl[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



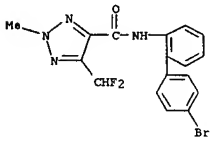
RN 668491-48-3 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-(4'-fluoro[1,1'-biphenyl]-2-yl)-2-methyl- (CA INDEX NAME)



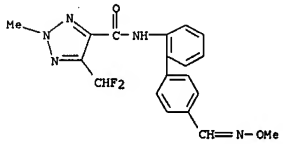
RN 668491-49-4 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-chloro[1,1'-biphenyl]-2-yl)-5-(difluoromethyl)-2-methyl- (CA INDEX NAME)



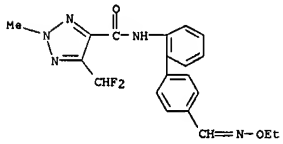
RN 668491-50-7 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-bromo[1,1'-biphenyl]-2-yl)-5-(difluoromethyl)-2-methyl- (CA INDEX NAME)



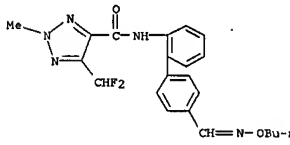
RN 668491-51-8 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-[4'-[(methoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl- (CA INDEX NAME)



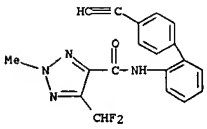
RN 668491-52-9 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-[4'-[(ethoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl- (CA INDEX NAME)



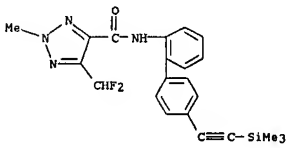
RN 668491-56-3 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-[4'-[(butoxyimino)methyl][1,1'-biphenyl]-2-yl]-5-(difluoromethyl)-2-methyl- (CA INDEX NAME)



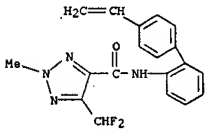
RN 668491-61-0 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-(4'-ethynyl[1,1'-biphenyl]-2-yl)-2-methyl- (CA INDEX NAME)



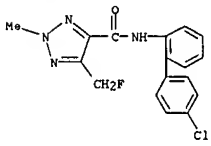
RN 668491-62-1 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-2-methyl-N-[4'-[(trimethylsilyl)ethynyl][1,1'-biphenyl]-2-yl]- (9CI) (CA INDEX NAME)



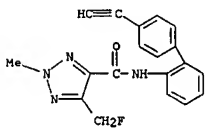
RN 668491-63-2 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-(4'-ethenyl[1,1'-biphenyl]-2-yl)-2-methyl- (CA INDEX NAME)



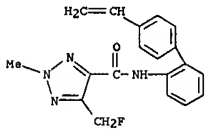
RN 668491-64-3 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-chloro[1,1'-biphenyl]-2-yl)-5-(fluoromethyl)-2-methyl- (CA INDEX NAME)



RN 668491-68-7 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethynyl[1,1'-biphenyl]-2-yl)-5-(fluoromethyl)-2-methyl- (CA INDEX NAME)



RN 668491-69-8 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethenyl[1,1'-biphenyl]-2-yl)-5-(fluoromethyl)-2-methyl- (CA INDEX NAME)



=> fil reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.01	358.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.56	-1.56

FILE 'REGISTRY' ENTERED AT 08:02:54 ON 29 NOV 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2
DICTIONARY FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

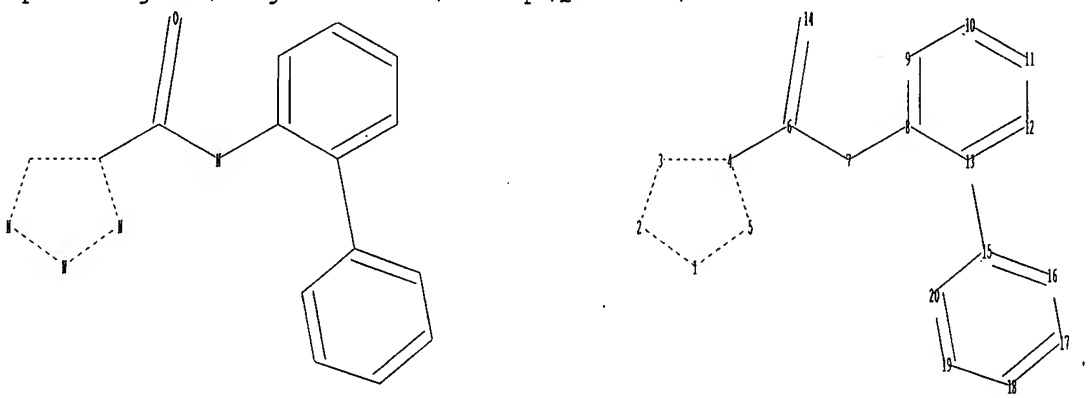
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10524721c.str



chain nodes :
6 7 14
ring nodes :
1 2 3 4 5 8 9 10 11 12 13 15 16 17 18 19 20
chain bonds :
4-6 6-7 6-14 7-8 13-15
ring bonds :
1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-14 7-8
exact bonds :
4-6 13-15
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom

L10 STRUCTURE UPLOADED

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.65	365.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.56

FILE 'REGISTRY' ENTERED AT 08:13:03 ON 29 NOV 2007

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2
DICTIONARY FILE UPDATES: 28 NOV 2007 HIGHEST RN 956214-95-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

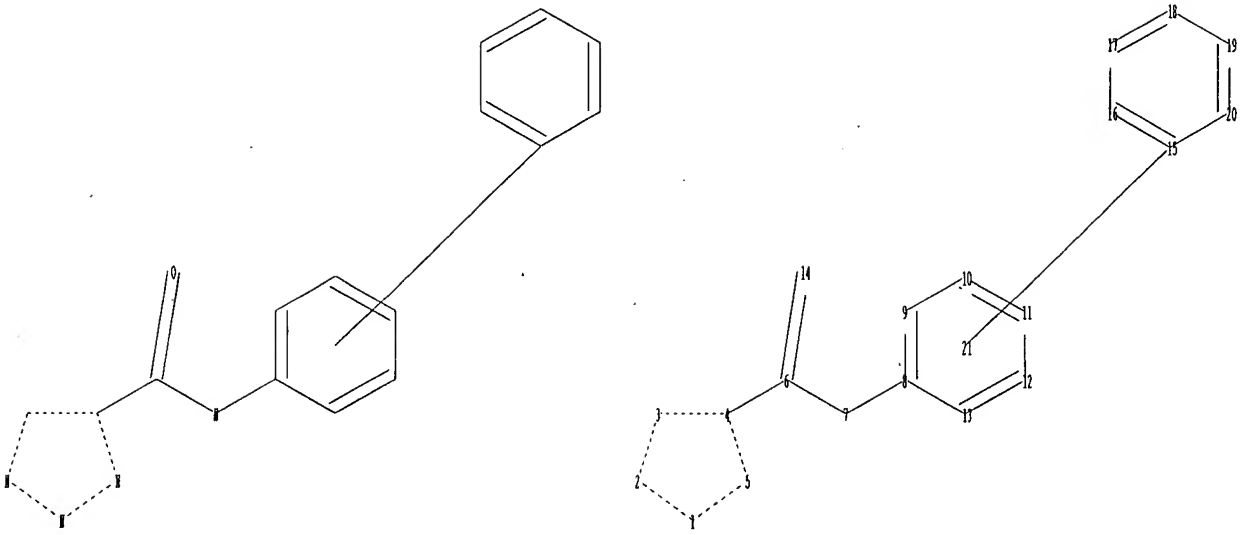
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10524721d.str

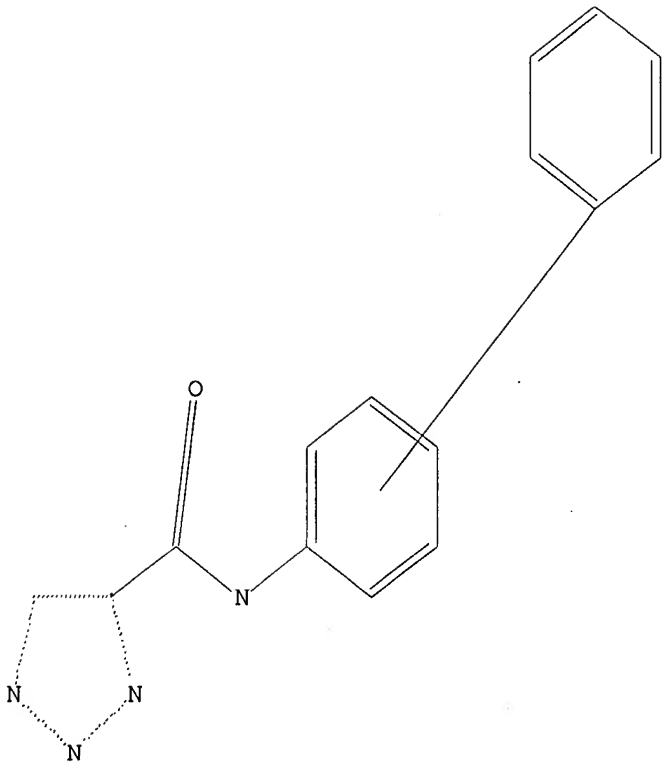


chain nodes :
6 7 14
ring nodes :
1 2 3 4 5 8 9 10 11 12 13 15 16 17 18 19 20
chain bonds :
4-6 6-7 6-14 7-8
ring bonds :
1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20 16-17
17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-14 7-8
exact bonds :
4-6
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom

L11 STRUCTURE UPLOADED

=> d
L11 HAS NO ANSWERS
L11 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s l11
SAMPLE SEARCH INITIATED 08:13:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      372 TO ITERATE

100.0% PROCESSED      372 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         6283 TO     8597
PROJECTED ANSWERS:               3 TO      163

L12           3 SEA SSS SAM L11

=> s l11 full
FULL SEARCH INITIATED 08:13:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     7056 TO ITERATE

100.0% PROCESSED     7056 ITERATIONS                               44 ANSWERS
SEARCH TIME: 00.00.01

L13          44 SEA SSS FUL L11

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
```

FULL ESTIMATED COST 172.10 537.97

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

CA SUBSCRIBER PRICE 0.00 -1.56

FILE 'CAPLUS' ENTERED AT 08:13:42 ON 29 NOV 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 29 Nov 2007 VOL 147 ISS 23
FILE LAST UPDATED: 28 Nov 2007 (20071128/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l13
L14 10 L13

=> d ibib abs hitstr tot

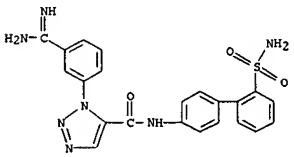
L14 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:511199 CAPLUS
DOCUMENT NUMBER: 143:145801
TITLE: Ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling
AUTHOR(S): Taha, Mutasem O.; Qandil, Amjad M.; Zaki, Dhia D.; AlDamen, Murad A.
CORPORATE SOURCE: Faculty of Pharmacy, Department of Pharmaceutical Sciences, University of Jordan, Amman, Jordan
SOURCE: European Journal of Medicinal Chemistry (2005), 40(7), 701-727
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The flexibility of activated factor X (fXa) binding site was assessed employing ligand-based pharmacophore modeling combined with genetic algorithm (GA)-based QSAR modeling. Four training subsets of wide structural diversity were selected from a total of 199 direct fXa inhibitors and were employed to generate different fXa pharmacophoric hypotheses using CATALYST software over two subsequent stages. In the first stage, high quality binding models (hypotheses) were identified. However, in the second stage, these models were refined by applying variable feature weight anal. to assess the relative significance of their features in the ligand-target affinity. The binding models were validated according to their coverage (capacity as a three-dimensional (3D) database search queries) and predictive potential as three-dimensional quant. structure-activity relationship (3D-QSAR) models. Subsequently, GA and multiple linear regression (MLR) anal. were employed to construct different QSAR models from high quality pharmacophores and explore the statistical significance of combination models in explaining bioactivity variations across 199 fXa inhibitors. Three orthogonal pharmacophoric models emerged in the optimal QSAR equation suggesting they represent three binding modes accessible to ligands in the binding pocket within fXa.

IT 209954-67-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling)

RN 209954-67-6 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)

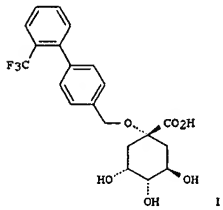


REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS

L14 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:441839 CAPLUS
DOCUMENT NUMBER: 143:153207
TITLE: Quinic Acid Derivatives as Sialyl Lewisx-Mimicking Selectin Inhibitors: Design, Synthesis, and Crystal Structure in Complex with E-Selectin
AUTHOR(S): Kaila, Neelu; Somers, William S.; Thomas, Bert E.; Thakker, Paresh; Janz, Kristin; DeBernardo, Silvano; Tam, Steve; Moore, William J.; Yang, Ruiyang; Wrona, Wojciech; Bedard, Patricia W.; Crommie, Deidre; Keith, James C., Jr.; Tsao, Desiree H. H.; Alvarez, Juan C.; Ni, Heyu; Marchese, Erik; Patton, John T.; Magnani, John L.; Camphausen, Raymond T.
CORPORATE SOURCE: Chemical Screening Sciences and Cardiovascular and Metabolic Disease Research, Wyeth, Cambridge, MA, 02140, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(13), 4346-4357
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:153207
GI



I

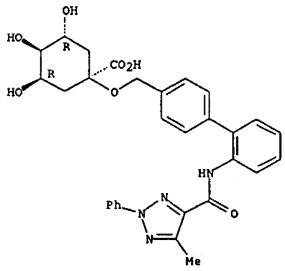
AB A search for noncarbohydrate sLex mimics led to the development of quinic acid derivs. as selectin inhibitors. At Wyeth the first cocrystal structure of a small mol., quinic acid, with E-selectin was solved. In the cocomplex two hydroxyls of quinic acid mimic the calcium-bound fucose of the tetrasaccharide sLex. The x-ray structure, together with structure based computational methods, was used to design quinic acid based libraries that were synthesized and evaluated for their ability to block the interaction of sLex with P-selectin. A large number of analogs were prepared using solution-phase parallel synthesis. Selected compds. showed decrease in leukocyte rolling in the IVM mouse model. I inhibited neutrophil influx in the murine TIP model and demonstrated good plasma exposure.

IT 859225-04-0P
RL: CPN (Combinatorial preparation); SPN (Synthetic preparation); CMBI (Combinatorial study); PREP (Preparation)
(preparation of a combinatorial library of quinic acid derivs. as sialyl Lewisx-mimicking selectin inhibitors including the design, and crystal

L14 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
structure in complex with E-selectin)

RN 859225-04-0 CAPLUS
CN Cyclohexanecarboxylic acid, 3,4,5-trihydroxy-1-[[2'-[[(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)carbonyl]amino][1,1'-biphenyl]-4-yl]methoxy]-, (3R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

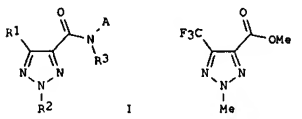
ACCESSION NUMBER: 2004:182852 CAPLUS
DOCUMENT NUMBER: 140:235719
TITLE: Preparation of triazolylcarboxylic acid derivatives with antifungal activity for agricultural use
INVENTOR(S): Ehrenfreund, Josef; Tobler, Hans; Walter, Harald
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018438	A2	20040304	WO 2003-EP9111	20030818
WO 2004018438	A3	20040826		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2494263	A1	20040304	CA 2003-2494263	20030818
AU 2003253417	A1	20040311	AU 2003-253417	20030818
EP 1539717	A2	20050615	EP 2003-792351	20030818
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003013686	A	20050621	BR 2003-13686	20030818
CN 1678593	A	20051005	CN 2003-819890	20030818
JP 2006502244	T	20060119	JP 2005-501204	20030818
EG 23485	A	20051205	EG 2003-821	20030820
IN 2004CN03147	A	20060217	IN 2004-CN3147	20041231
MX 2005PA01819	A	20050419	MX 2005-PA1819	20050215
US 2006154967	A1	20060713	US 2005-524721	20050216

PRIORITY APPLN. INFO.:

GB 2002-19612	A	20020822
GB 2003-10464	A	20030507
WO 2003-EP9111	W	20030818

OTHER SOURCE(S): MARPAT 140:235719
GI

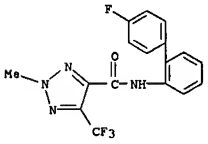


I II

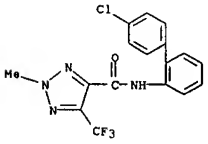
AB Title compds. I [A = ortho-substituted aryl or heteroaryl ring system; R1 = halo, CN, NO2, alkyl, haloalkyl, alkoxy, haloalkoxy, (un)substituted alkene, etc.; R2 = alkyl, haloalkyl, alkoxyalkyl, etc.; R3 = H, (un)substituted-alkyl, -propargyl, -alkoxy, etc.] were prepd. and disclosed as having antifungal activity. Thus, e.g., II was prepd. via methylation of 1,2,3-triazole-4,5-dicarboxylic acid di-Me ester, with subsequent monohydrolysis and fluorination of the carboxylic acid moiety to the trifluoromethyl moiety. I were tested against 9 different agriculturally relevant fungi with varying degrees of efficacy obsd. Addnl., a compn. of I with a suitable carrier for controlling microorganisms and preventing attack and infestation of plants therewith is claimed.

IT 668491-33-6P 668491-34-7P 668491-35-8P
668491-36-9P 668491-37-0P 668491-45-0P
668491-46-1P 668491-47-2P 668491-48-3P
668491-49-4P 668491-50-7P 668491-51-8P
668491-52-9P 668491-56-3P 668491-61-0P
668491-62-1P 668491-63-2P 668491-64-3P
668491-68-7P 668491-69-8P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of triazolylcarboxylic acid derivs. with antifungal activity)

RN 668491-33-6 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-fluoro[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)

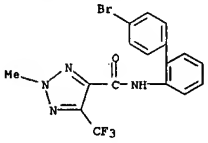


RN 668491-34-7 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-chloro[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)

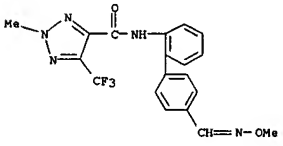


RN 668491-35-8 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-bromo[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)

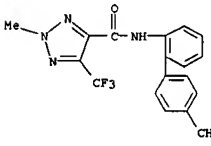
L14 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 668491-36-9 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-[4'-[(methoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)

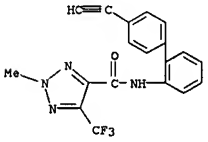


RN 668491-37-0 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-[4'-[(ethoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)

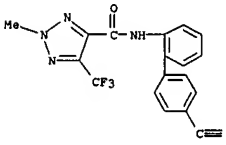


RN 668491-45-0 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethynyl[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)

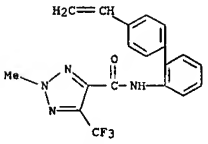
L14 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



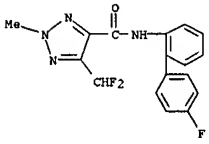
RN 668491-46-1 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 2-methyl-5-(trifluoromethyl)-N-[4'-[(trimethylsilyl)ethynyl][1,1'-biphenyl]-2-yl]- (9CI) (CA INDEX NAME)



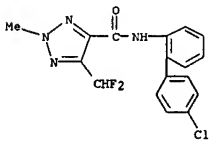
RN 668491-47-2 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethenyl[1,1'-biphenyl]-2-yl)-2-methyl-5-(trifluoromethyl)- (CA INDEX NAME)



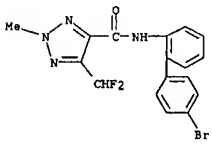
RN 668491-48-3 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-(4'-fluoro[1,1'-biphenyl]-2-yl)-2-methyl- (CA INDEX NAME)



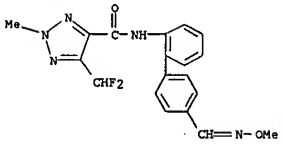
RN 668491-49-4 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-chloro[1,1'-biphenyl]-2-yl)-5-(difluoromethyl)-2-methyl- (CA INDEX NAME)



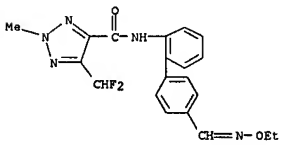
RN 668491-50-7 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-bromo[1,1'-biphenyl]-2-yl)-5-(difluoromethyl)-2-methyl- (CA INDEX NAME)



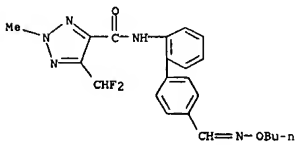
RN 668491-51-8 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-[4'-[(methoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl- (CA INDEX NAME)



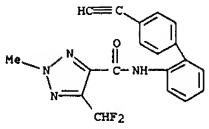
RN 668491-52-9 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-[4'-[(ethoxyimino)methyl][1,1'-biphenyl]-2-yl]-2-methyl- (CA INDEX NAME)



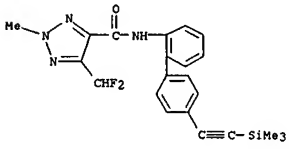
RN 668491-56-3 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-[4'-[(butoxyimino)methyl][1,1'-biphenyl]-2-yl]-5-(difluoromethyl)-2-methyl- (CA INDEX NAME)



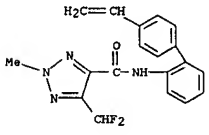
RN 668491-61-0 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-(4'-ethynyl[1,1'-biphenyl]-2-yl)-2-methyl- (CA INDEX NAME)



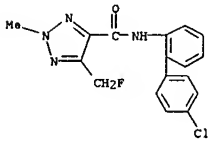
RN 668491-62-1 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-2-methyl-N-[4'-[(trimethylsilyl)ethynyl][1,1'-biphenyl]-2-yl]- (9CI) (CA INDEX NAME)



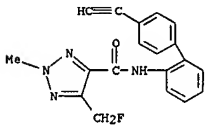
RN 668491-63-2 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, 5-(difluoromethyl)-N-(4'-ethenyl[1,1'-biphenyl]-2-yl)-2-methyl- (CA INDEX NAME)



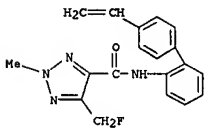
RN 668491-64-3 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-chloro[1,1'-biphenyl]-2-yl)-5-(fluoromethyl)-2-methyl- (CA INDEX NAME)



RN 668491-68-7 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethynyl[1,1'-biphenyl]-2-yl)-5-(fluoromethyl)-2-methyl- (CA INDEX NAME)



RN 668491-69-8 CAPLUS
CN 2H-1,2,3-Triazole-4-carboxamide, N-(4'-ethenyl[1,1'-biphenyl]-2-yl)-5-(fluoromethyl)-2-methyl- (CA INDEX NAME)



L14 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:522631 CAPLUS
DOCUMENT NUMBER: 137:93747
TITLE: Preparation of pyrazolecarboxamides as inhibitors of factor Xa
INVENTOR(S): Zhu, Bing-yan; Jia, Zhaozhong Jon; Huang, Wenrong; Song, Yonghong; Kanter, James; Scarborough, Robert M.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 303 pp., Cont.-in-part of U.S. Ser. No. 662,807.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20020091116	A1	20020711	US 2001-794214	20010228
US 6632815	B2	20031014		
US 6720317	B1	20040413	US 2000-662807	20000915
US 6686368	B1	20040203	US 2003-387927	20030312
US 2004116399	A1	20040617	US 2003-600695	20030620
US 2006020039	A1	20060126	US 2005-35767	20050114
US 7285565	B2	20071023		
PRIORITY APPLN. INFO.:			US 1999-154332P	P 19990917
			US 2000-662807	A2 20000915
			US 2000-185746P	P 20000229
			US 2000-663420	A1 20000915
			US 2001-794214	A1 20010228

OTHER SOURCE(S): MARPAT 137:93747
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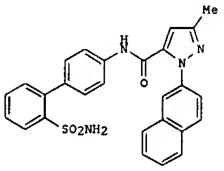
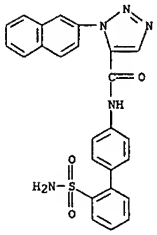


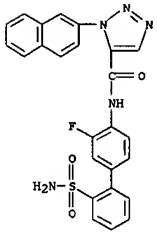
I

AB The title compds. AQDEGJX [A = alkyl, cycloalkyl, (un)substituted Ph, naphthyl, etc.; Q = a direct link, divalent alkyl, alkenyl, etc.; D = a direct link, (un)substituted Ph, 5-10 membered (non)aromatic heterocyclyl; E = a direct link, (CH2)qCO, CO(CH2)x, etc.; q, x = 0-2; G = (un)substituted Ph, 5-6 membered heteroaryl; J = a direct link, SO2, CO, etc.; X = (un)substituted Ph, naphthyl, 6-membered heteroaryl, etc.] having activity against mammalian factor Xa, and useful in vitro or in vivo for preventing or treating coagulation disorders, were prepared E.g., a 3-step synthesis of the pyrazolecarboxamide I was given.
IT 441328-78-5P 441328-79-6P

L14 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrazolecarboxamides as inhibitors of factor Xa)
RN 441328-78-5 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1-(2-naphthalenyl)- (CA INDEX NAME)



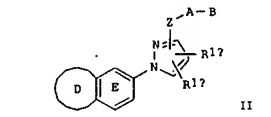
RN 441328-79-6 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-1-(2-naphthalenyl)- (CA INDEX NAME)



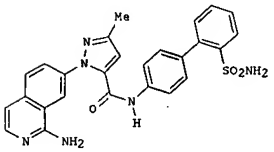
L14 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:39605 CAPLUS
DOCUMENT NUMBER: 136:102380
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John M.; Han, Qi; Li, Renhua; Pinto, Donald J. P.; Pruitt, James R.; Quan, Mimi L.
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: U.S., 117 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6339099	B1	20020115	US 1998-99358	19980618
US 2002025963	A1	20020228	US 2001-924381	20010808
US 6906070	B2	20050614		
US 2003069258	A1	20030410	US 2002-98994	20020313
US 6958356	B2	20051025		
US 2004063772	A1	20040401	US 2003-602214	20030624
US 6965036	B2	20051115		
US 2006040973	A1	20060223	US 2005-197978	20050805
US 7235575	B2	20070626		
PRIORITY APPLN. INFO.:			US 1997-50265P	P 19970620
			US 1998-99358	A3 19980618
			US 2001-924381	B1 20010808
			US 2002-98994	A1 20020313

OTHER SOURCE(S): MARPAT 136:102380
GI



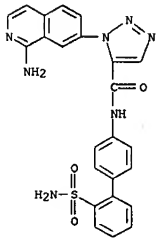
II



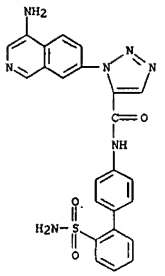
II

AB The title compds. [I; ring D = 5-membered aromatic system containing from 1-2

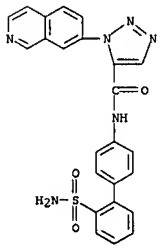
L14 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
heteroatoms selected from N, O, S; ring D is substituted with 0-2 R groups; ring E contains 0-2 N atom and is substituted by 0-1 R groups; R = Cl, F, Br, I, OH, alkoxy, amino(alkyl), (alkyl)amino; Z = bond, alkylene, (CH2)rO(CH2)r, (CH2)rNR3(CH2)r, (CH2)rC(O)(CH2)r, (CH2)rC(O)O(CH2)r, (CH2)rOC(O)(CH2)r, (CH2)rC(O)NR3(CH2)r, etc. provided that Z does not form a N-N, N-O, N-S, NCH2N, NCH2O, or NCH2S bond with ring M or group A; R1a-1b = H, alk(en)yl, aminoalkyl, alkoxy, alternatively, R1a-1b, when attached to adjacent carbon atoms, together with the atoms to which they are attached form a 5-8 membered (un)satd. ring (un)substituted and which contains from 0-2 heteroatoms selected from the group consisting of N, O, and S; alternatively, when Z is C(O)NH and R1a is attached to a ring carbon adjacent to Z, then R1a is a C(O) which replaces the amide hydrogen of Z to form a cyclic imide; R3 = H, alkyl, phenyl; A = (un)substituted carbocyclic, 5-10 membered heterocyclic system contg. 1-4 heteroatoms selected from N, O, S; B = H, Y, X-Y; X = sulfonylalkyl, alkylsulfonyl, sulfonamide, etc.; Y = alkylamino, provided that X-Y does not form a N-N, O-N or S-N bond, carbocyclic group, 5-10 membered heterocyclic r = 0-3], inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepd. and formulated. Thus, a multi-step synthesis of the title compd. II, starting with 7-aminoisoquinoline, was described. A no. of compds. I were found to exhibit a Ki of ≤ 15 μM against factor Xa.
IT 218297-96-2P 218297-97-3P 218297-98-4P
218299-21-9P 218299-22-0P 218301-03-2P
218301-04-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel guanidine mimics as factor Xa inhibitors)
RN 218297-96-2 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



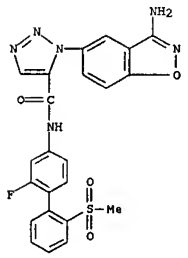
RN 218297-97-3 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(4-amino-7-isoquinolinyl)-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



RN 218297-98-4 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1-(7-isoquinolinyl)- (CA INDEX NAME)



RN 218299-21-9 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



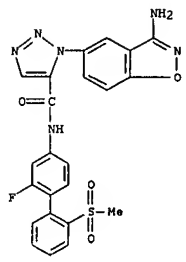
CM 2

CRN 76-05-1
CMF C2 H F3 O2

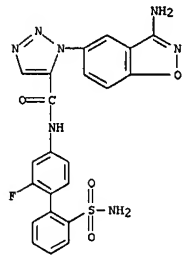
RN 218301-04-3 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2'-(aminosulfonyl)-2-fluoro[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 218299-22-0
CMF C22 H16 F N7 O4 S



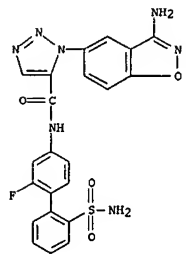
RN 218299-22-0 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2'-(aminosulfonyl)-2-fluoro[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



RN 218301-03-2 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 218299-21-9
CMF C23 H17 F N6 O4 S

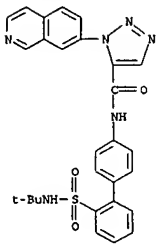


CM 2

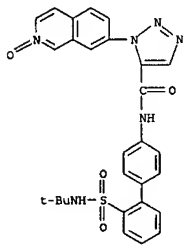
CRN 76-05-1
CMF C2 H F3 O2

IT 218301-44-1P 218301-45-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel guanidine mimics as factor Xa inhibitors)
RN 218301-44-1 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1-(7-isoquinolinyl)- (CA INDEX NAME)

L14 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 218301-45-2 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1-(2-oxido-7-isoquinolinyl)- (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:177435 CAPLUS
DOCUMENT NUMBER: 135:40405
TITLE: Synthesis and SAR of benzamidine factor Xa inhibitors containing a vicinally-substituted heterocyclic core
AUTHOR(S): Fevig, J. M.; Pinto, D. J.; Han, Q.; Quan, M. L.; Pruitt, J. R.; Jacobson, I. C.; Galemmo, R. A., Jr.; Wang, S.; Orwat, M. J.; Bostrom, L. L.; Knabb, R. M.; Wong, P. C.; Lam, P. Y. S.; Wexler, R. R.
CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(5), 641-645
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:40405

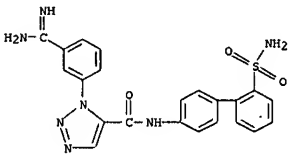
AB The selective inhibition of coagulation factor Xa has emerged as an attractive strategy for the discovery of novel antithrombotic agents. Here we describe highly potent benzamidine factor Xa inhibitors based on a vicinally-substituted heterocyclic core.

IT 344416-70-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and SAR of benzamidine factor Xa inhibitors containing a vicinally-substituted heterocyclic core)

RN 344416-70-2 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-67-6
CMF C22 H19 N7 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L14 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

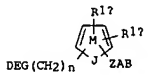
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:83115 CAPLUS
DOCUMENT NUMBER: 132:137392
TITLE: Preparation of azoles as Factor Xa inhibitors.
INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Co., USA
SOURCE: U.S., 152 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6020357	A	20000201	US 1997-995834	19971222
US 6548512	B1	20030415	US 2000-492708	20000127
PRIORITY APPLN. INFO.:			US 1996-33437P P	19961223
			US 1997-50304P P	19970620
			US 1997-995834 A3	19971222

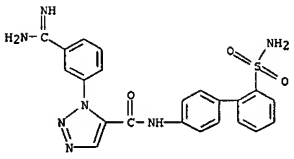
OTHER SOURCE(S): MARPAT 132:137392
GI



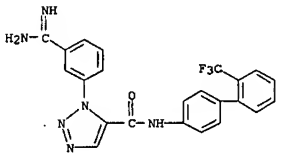
AB Title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2; with provisos], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded 1-(3-amidinophenyl)-2-[(2'-aminosulfonyl-1,1'-biphen-4-yl)aminocarbonyl]imidazole. Several I showed Ki ≤10 μM against Factor Xa and thrombin.

IT 209954-67-6P 209955-00-0P 209957-70-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azoles as Factor Xa inhibitors)

RN 209954-67-6 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



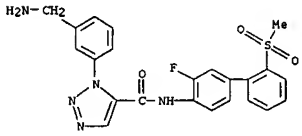
RN 209955-00-0 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



RN 209957-70-0 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

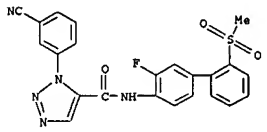
CRN 209957-69-7
CMF C23 H20 F N5 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 209960-21-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azoles as Factor Xa inhibitors)
RN 209960-21-4 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-cyanophenyl)-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



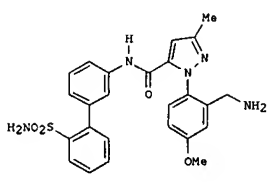
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1999:421659 CAPLUS
DOCUMENT NUMBER: 131:58820
TITLE: Preparation of nitrogen heteroaromatics as blood coagulation factor Xa inhibitors
INVENTOR(S): Galemmo, Robert A., Jr.; Pinto, Donald J. P.; Bostrom, Lori L.; Rossi, Karen Anita
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 237 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9932454	A1	19990701	WO 1998-US26427	19981211
W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2314401	A1	19990701	CA 1998-2314401	19981211
AU 9917244	A	19990712	AU 1999-17244	19981211
BR 9813835	A	20001010	BR 1998-13835	19981211
EP 1042299	A1	20001011	EP 1998-962082	19981211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
JP 2001526268	T	20011218	JP 2000-525391	19981211
ZA 9811517	A	20000615	ZA 1998-11517	19981215
US 6271237	B1	20010807	US 1998-217336	19981221
MX 2000PA06159	A	20011011	MX 2000-PA6159	20000621
US 2002016326	A1	20020207	US 2001-833302	20010412
US 6548525	B2	20030415		

PRIORITY APPLN. INFO.:
US 1997-68491P P 19971222
US 1997-996447 A 19971222
US 1998-101075P P 19980918
WO 1998-US26427 W 19981211
US 1998-217336 A3 19981221

OTHER SOURCE(S): MARPAT 131:58820
GI

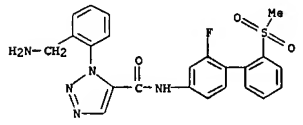


II

AB DEG(CH2)sMZAB [I; D = cyano, amino(alkyl), amidino, etc.; E =

(un)substituted phenylene, -pyridinediyl, -pyrimidinediyl, etc.; G = bond, NHCH2, OCH2, SCH2; M = (un)substituted pyrrolylene, -di-, -tri-, or -tetrazolylene; Z = (heteroatom-interrupted)(oxo)alkylene, oxyalkylene, alkyleneoxy, etc.; A = (un)substituted carbocyclic residue (sic) or -heterocyclylene; B = amino(alkyl), amidino, ureido, (un)substituted carbocyclic residue, etc.; s = 0-2] were prepd. Thus, 2-hydrazino-5-methoxybenzoic acid was cyclocondensed with MeCOCH2C(:NOMe)CO2Et (prepn. each given) and the product converted in 3 steps to 3-methyl-1-(2-azidomethyl-4-methoxyphenyl)-1H-pyrazole-5-carboxylic acid which was amidated by 4-(H2N)C6H4C6H4(CO2NHCMe3)-2 to give, in 2 addnl. steps, title compd. II. Data for biol. activity of I were given.

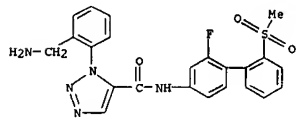
IT 228258-55-7P 228258-95-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)
RN 228258-55-7 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



RN 228258-95-5 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-55-7
CMF C23 H20 F N5 O3 S



CM 2

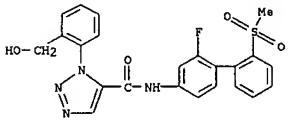
CRN 76-05-1

CMF C2 H F3 O2

IT 228259-58-3P 228259-59-4P 228259-60-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)

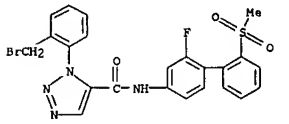
RN 228259-58-3 CAPLUS

CN 1H-1,2,3-Triazole-5-carboxamide, N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-(hydroxymethyl)phenyl]- (CA INDEX NAME)



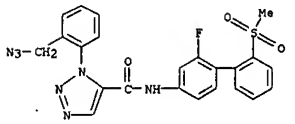
RN 228259-59-4 CAPLUS

CN 1H-1,2,3-Triazole-5-carboxamide, 1-[2-(bromomethyl)phenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



RN 228259-60-7 CAPLUS

CN 1H-1,2,3-Triazole-5-carboxamide, 1-[2-(azidomethyl)phenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1999:9833 CAPLUS
DOCUMENT NUMBER: 130:66494
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John Matthew; Han, Qi; Li, Renhua; Pinto, Donald Joseph-Phillip; Pruitt, James Russell; Quan, Mimi Lifen
PATENT ASSIGNEE(S): The Du Pont Merck Pharmaceutical Company, USA
SOURCE: PCT Int. Appl., 268 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9857951	A1	19981223	WO 1998-US12680	19980618
W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9805247	A	19991217	ZA 1998-5247	19980617
CA 2291442	A1	19981223	CA 1998-2291442	19980618
AU 9879768	A	19990104	AU 1998-79768	19980618
AU 756755	B2	20030123		
EP 991638	A1	20000412	EP 1998-930361	19980618
EP 991638	B1	20050817		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
BR 9810137	A	20000808	BR 1998-10137	19980618
EE 9900583	A	20000815	EE 1999-583	19980618
EE 4153	B1	20031015		
HU 2000002686	A2	20020128	HU 2000-2686	19980618
HU 2000002686	A3	20020228		
JP 2002505686	T	20020219	JP 1999-504785	19980618
NZ 502370	A	20021025	NZ 1998-502370	19980618
AT 302198	T	20050915	AT 1998-930361	19980618
ES 2244064	T3	20051201	ES 1998-930361	19980618
RO 120543	B1	20060330	RO 1999-1317	19980618
PL 192941	B1	20061229	PL 1998-337756	19980618
SK 285685	B6	20070607	SK 1999-1728	19980618
TW 544453	B	20030801	TW 1998-87109910	19980819
NO 9905965	A	19991203	NO 1999-5965	19991203
NO 318359	B1	20050307		
MX 9911908	A	20000531	MX 1999-11908	19991216
LV 12496	B	20010120	LV 1999-178	19991216
LT 4705	B	20000925	LT 1999-147	19991217
PRIORITY APPLN. INFO.:			US 1997-878884 A	19970619
			WO 1998-US12680 W	19980618

OTHER SOURCE(S): MARPAT 130:66494
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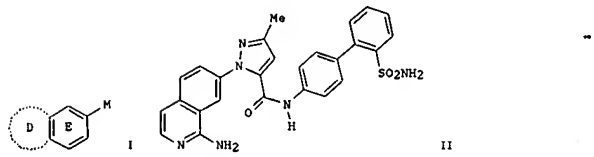
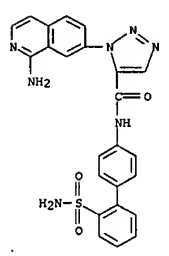


AB The title compds. {I; rings D-E represent guanidine mimics; ring D = CH2N:CH, CH2CH2N:CH, a 5-6 membered aromatic system containing 0-2 heteroatoms selected form the group N, O, and S; ring D is substituted with 0-2 R (substituents), provided that when ring D is unsubstituted, it contains at least one heteroatom; ring E contains 0-2 N atom and is substituted by 0-1 R; R = halo, OH, C1-3 alkoxy, etc.; M = (un)substituted pyrazole, imidazole, tetrazole, etc.], inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step synthesis of the title compound II, starting with 7-aminoisoquinoline, was described. A number of compds. I were found to exhibit a Ki of ≤ 15 μM against factor Xa.

IT 218297-96-2P 218297-97-3P 218297-98-4P
218299-21-9P 218299-22-0P 218301-03-2P
218301-04-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel guanidine mimics as factor Xa inhibitors)

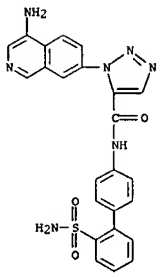
RN 218297-96-2 CAPLUS

CN 1H-1,2,3-Triazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)

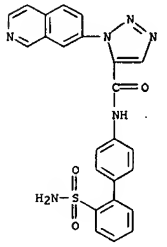


RN 218297-97-3 CAPLUS

L14 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(4-amino-7-isoquinolinyl)-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)

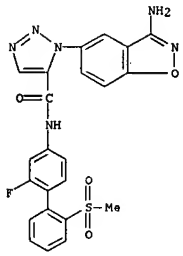


RN 218297-98-4 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1-(7-isoquinolinyl)- (CA INDEX NAME)

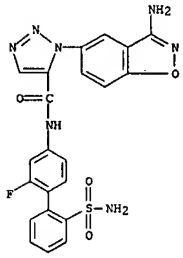


RN 218299-21-9 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)

L14 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 218299-22-0 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2'-(aminosulfonyl)-2-fluoro[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)

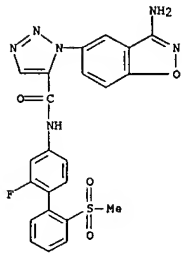


RN 218301-03-2 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 218299-21-9
CMF C23 H17 F N6 O4 S

L14 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

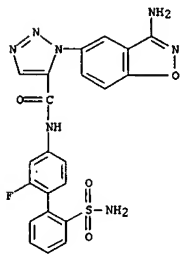
CRN 76-05-1
CMF C2 H F3 O2

RN 218301-04-3 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2'-(aminosulfonyl)-2-fluoro[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 218299-22-0
CMF C22 H16 F N7 O4 S

L14 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

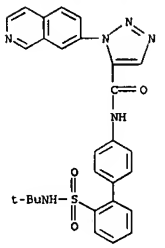


CM 2

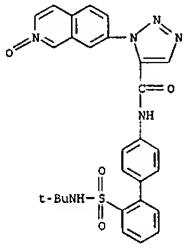
CRN 76-05-1
CMF C2 H F3 O2

IT 218301-44-1P 218301-45-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel guanidine mimics as factor Xa inhibitors)
RN 218301-44-1 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1-(7-isoquinolinyl)- (CA INDEX NAME)

L14 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 218301-45-2 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-1-(2-oxido-7-isoquinolinyl)- (CA INDEX NAME)

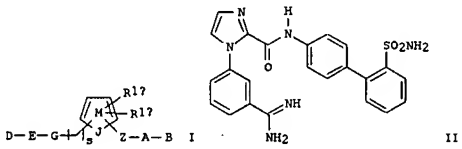


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:479506 CAPLUS
DOCUMENT NUMBER: 129:109090
TITLE: Preparation of nitrogen-containing heteroaromatics as factor Xa inhibitors
INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita
PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Co., USA
SOURCE: PCT Int. Appl., 438 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

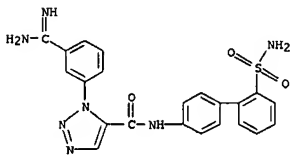
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9828269	A1	19980702	WO 1997-US22895	19971215
W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2275796	A1	19980702	CA 1997-2275796	19971215
AU 9856020	A	19980717	AU 1998-56020	19971215
AU 730224	B2	20010301		
EP 946508	A1	19991006	EP 1997-952409	19971215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
EE 9900316	A	20000215	EE 1999-316	19971215
SI 20017	A	20000229	SI 1997-20082	19971215
CN 1246847	A	20000308	CN 1997-181852	19971215
BR 9714073	A	20000509	BR 1997-14073	19971215
HU 2000000735	A2	20010428	HU 2000-735	19971215
HU 2000000735	A3	20020328		
JP 2001509145	T	20010710	JP 1998-528845	19971215
ZA 9711586	A	19990701	ZA 1997-11586	19971223
TW 492971	B	20020701	TW 1997-86119637	19980203
NO 9902633	A	19990820	NO 1999-2633	19990601
NO 313190	B1	20020826		
MX 9905878	A	20000131	MX 1999-5878	19990622
LT 4673	B	20000725	LT 1999-76	19990622
LV 12430	B	20000720	LV 1999-99	19990730

PRIORITY APPLN. INFO.: US 1996-769859 A 19961223; US 1997-879944 A 19970620; WO 1997-US22895 W 19971215
OTHER SOURCE(S): MARPAT 129:109090
GI .

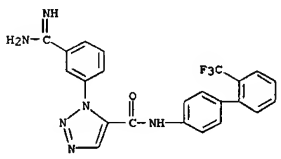


I II

L14 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
AB The title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded the title compound II. A number of compds. I were found to exhibit a Ki of ≤ 10 μM against factor Xa. Some compds. I were evaluated and found to exhibit Ki of < 10 μM against thrombin.
IT 209954-67-6P 209955-00-0P 209957-69-7P
209957-70-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)
RN 209954-67-6 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)

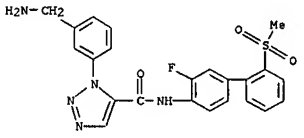


RN 209955-00-0 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



RN 209957-69-7 CAPLUS

L14 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



RN 209957-70-0 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 209957-69-7
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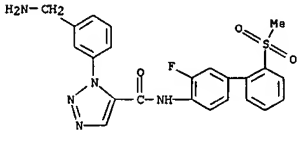
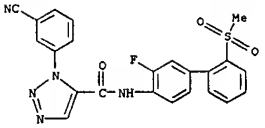


CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 209960-21-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)
RN 209960-21-4 CAPLUS
CN 1H-1,2,3-Triazole-5-carboxamide, 1-(3-cyanophenyl)-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	64.92	602.89

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.80	-9.36

STN INTERNATIONAL LOGOFF AT 08:29:10 ON 29 NOV 2007